Trapped Particles in PT Symmetric Theories

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Abstract

PT symmetric quantum mechanics for a particle trapped by the generalized non-Hermitian harmonic oscillator potential is studied. It is shown that energy and the expectation value of the position operator x can not be real simultaneously, if the particle is trapped. Non-vanishing boundary conditions for the trapped particle in PT symmetric theory are also discussed.

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I. INTRODUCTION

It is commonly believed that the Hamiltonian must be hermitian in order to ensure that the energy spectrum is real and that the time evolution of the theory is unitary. Although this axiom is necessary to guarantee these desired properties, the recent studies have shown that it is not sufficient [1, 2, 3, 4, 5, 6, 7]. It is shown that there is a simpler and more physical alternative axiom to Hermicity. It is the space-time reflection symmetry (PT symmetry). The Hamiltonans may not be symmetric under P or T separately, It should be invariant under their combined operation.

The first examples for complex potentials with real spectra were found by using the numerical techniques. After the first examples, further ones have been identified using perturbative technique [8] and some exactly solvable PT symmetric Hamiltonians [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19] have been found. Exactly solvable examples are extremely useful in the understanding of unusual features of PT symmetric problems and the underlying new physical concepts. It is a promising development, with possible applications ranging from the field theories [20, 21] to the supersymmetric models [22, 23].

Since PT symmetry is an alternative condition to Hermicity, it is now possible to construct infinitely many new Hamiltonians that would have been rejected before because they are not Hermitian.

Let us recall the properties of PT operation. The parity operator is linear and has the effect

$$p \to -p, \qquad x \to -x. \tag{1}$$

The time-reversal operator is antilinear and has the effect

$$p \to -p, \qquad x \to x, \qquad i \to -i. \tag{2}$$

Note that the Heisenberg algebra $[x, p] = i$ is preserved since T changes the sign of i.

In recent times, it has been found that in contrast with the first conjectures, neither Hermicity nor PT symmetry serves as a sufficient condition for a quantum Hamiltonian to preserve the reality of energy eigenvalues [24, 25, 26, 27, 28, 29]. In fact, it has been realized that the existence of real eigenvalues can be associated with a non-Hermitian Hamiltonian provided it is η-pseudo Hermitian $H^\dagger = \eta H \eta^{-1}$. In this context, PT symmetry is P-pseudo-Hermicity for one dimensional Hamiltonians.

There are more than one method to study the non-Hermitian Hamiltonian with the real spectra. One of the methods is to generate the non-Hermitian Hamiltonian from the corresponding Hermitian Hamiltonian by a complex shift of coordinate $x \to x - ic$, where c is a constant. For example, with this imaginary coordinate shift, the harmonic oscillator Hamiltonian becomes non-hermitian Hamiltonian giving the real energy spectrum [19].

In this study, we aim at whether confinement of a particle leads to the new physical implications in PT symmetric theories. To study this phenomenon, so-called complex shift of coordinate method will be utilized. Here, our motivation is to investigate whether the energy eigenvalues remain real if the particle is trapped into a box, namely, the wave function which vanishes at a finite point. The generalized harmonic oscillator potential is chosen for our study since the exact solutions are also well-known for this boundary conditions.

This paper is organized as follows. In the following section, the exact solution for the trapped particle under the generalized harmonic oscillator potential will be reviewed. In the last section, the imaginary coordinate shift will be applied both to the Hamiltonian to generate the non-Hermitian one and to the wave function to check the reality of energy eigenvalues.

II. FORMALISM

In this section, we review the exact solution for the trapped particle under the generalized harmonic oscillator potential [30]. The confinement of a particle plays an important role in the application of the quantum theory. For example, the electrons in a semiconductor are confined by a potential well in 1D (quantum well), 2D (quantum wire), or 3D (quantum dot). As a first approximation, these materials can be understood from a particle in a box perspective. Trapping it in a small space means that only particular types of wave-function are allowed. These wave-functions have each a particular characteristic length as well as a particular energy. Note that as the box size reduces the energy spacing changes. Hence one may expect that the extent of confinement changes the spectroscopic properties of quantum dots. Because of the wide application of confinement, PT symmetric version of confinement phenomena is worthy studying.

The generalized harmonic oscillator potential is of great significance in understanding the new physical effects of PT symmetric quantum theory since it can be solvable analytically.

It is of harmonic plus inverse harmonic type. The corresponding Schrodinger equation for this potential reads

$$-\frac{\partial^2\Psi}{\partial x^2}+\left(\omega^2(t)x^2+\frac{g}{x^2}\right)\Psi=i\frac{\partial\Psi}{\partial t}\ , \tag{3}$$

where angular frequency $\omega^2(t)$ is in general taken to be time-dependent and g is the coupling constant. The constants in Schrodinger equation are set to unity for simplicity $(\frac{\hbar^2}{2m}=\hbar=1)$.

Firstly, to find the exact confined solution of the problem, the following transformation on the wave function is introduced.

$$\Psi(x,t)=\exp\left(\ i\alpha\frac{x^2}{2}-\int_0^t dt'\alpha(t')\ \right)\Phi(x,t)\ . \tag{4}$$

where $\alpha(t)$ is to be determined later. If we apply this transformation into the Schrodinger equation, we get

$$-\frac{\partial^2\Phi}{\partial x^2}-2i\alpha x\frac{\partial\Phi}{\partial x}+\frac{g}{x^2}\Phi=i\frac{\partial\Phi}{\partial t}\ , \tag{5}$$

Here, $\alpha(t)$ is assumed to satisfy the following relation to get rid of the quadratic term in the above equation

$$\omega^2+\frac{\dot{\alpha}}{2}+\alpha^2=0\ . \tag{6}$$

The solution to this equation determines $\alpha(t)$. Now, we aim at solving the equation (5). To do this, the coordinate is scaled by a time-dependent function $L(t)$. The relation between the coordinate x and the new coordinate q is introduced as follows

$$x\rightarrow q=\frac{x}{L(t)}\ , \tag{7}$$

with a consequent transformation for the time derivative operator which is given by $\partial/\partial t\rightarrow\partial/\partial t-(\dot{L}/L)\ q\ \partial/\partial q$, where dot denotes time derivation. We have a freedom to choose $L(t)$. Let $L(t)$ be chosen as follows.

$$2\alpha=\frac{\dot{L}}{L}\ . \tag{8}$$

Instead of dealing with the relation between the time-dependent functions $L(t)$ and $\alpha(t)$, it is useful to study with the relation between $L(t)$ and $\omega^2(t)$. It can be computed by using the equations (6,8)

$$4\omega^2=-\frac{\ddot{L}}{L}\ . \tag{9}$$

The equation (5) become time-independent and includes only the inverse harmonic oscillator potential

$$-\frac{\partial^2\Phi(q)}{\partial q^2}+\left(\frac{g}{q^2}\right)\Phi(q)=E\Phi(q). \tag{10}$$

In the last step, we used the separation of variables technique. It is given by

$$\Phi(q,t)=\exp\left(-i\int_0^t dt'\frac{E}{L^2}\right)\Phi(q)\ , \tag{11}$$

where E is the constant and it does not coincide with the energy eigenvalues in general since $L(t)$ is time-dependent in general.

The equation (10) is a well known equation in physics and it's solution can be found easily. It is given by

$$\Phi(q)=q^{1/2}J_\nu(\sqrt{E}\ q)\ , \tag{12}$$

where $\nu=\frac{1}{2}(1+4g)^{1/2}$ and J_v is the Bessel function. The confined solution is given in term of the Bessel function which vanishes at some points. Transforming backwards yields the exact wave function for the generalized harmonic oscillator

$$\Psi_\nu(x,t)=N\exp\left(\ i\alpha\frac{x^2}{2}-i\int_0^t dt'\frac{E}{L^2}\ \right)\frac{1}{\sqrt{L}}\ R_\nu(x,t)\ , \tag{13}$$

where N is a normalization constant and $R_\nu(x,t)$ is given by

$$R_\nu(x,t)=\left(\frac{x}{L}\right)^{1/2}J_\nu\left(\sqrt{E}\ \frac{x}{L}\right)\ . \tag{14}$$

In the equation (13) we used the relation, $\frac{1}{\sqrt{L}}=\exp\left(-\int_0^t\alpha dt'\right)$ by (8). Bessel function is used in the solution of the generalized harmonic oscillator potential. Since Bessel function is zero at some finite points, it describes the trapped particle from the physical point of view. Now, let us make some remarks on the boundary conditions. Since Bessel function includes the time dependent function $L(t)$, the boundary condition is not stationary anymore. In general, it is a moving boundary condition. Bessel function in the equation (14) represents trapped particle into the box whose wall moves. For example, if $\omega^2(t)$ is constant, then $L(t)$ is sinusoidal by (9).

Having obtained the exact solution, let us write the new boundary conditions.

$$\Psi(x=L(t),t)=0\Rightarrow\Phi(q=1,t)=0\ ;\qquad \Psi(x=0,t)=0\Rightarrow\Phi(q=0,t)=0\ . \tag{15}$$

The time-dependent function $L(t)$ which determines boundary of the trap can not be chosen completely free. It depends on the time dependent character of $\omega^2(t)$. As can be seen from

the boundary condition (15), the particle is confined into a box whose wall moves with the speed $\dot{L}(t)$. To satisfy the boundary condition (15), the constant E takes discrete values. These values are the roots of the Bessel function $J_\nu(\sqrt{E})$ for a given value of ν.
Although the exact solution can be constructed only for some special choice of $L(t)$, it's implications turns out to be quite useful in understanding of PT symmetric quantum theory as can be seen in the next section.
Having obtained the exact solutions corresponding the two different boundary conditions, let us apply the complex shift of coordinate method to study PT symmetric extension of generalized harmonic oscillator problem.

III. COMPLEX SHIFT OF COORDINATE

It is of great importance to understand the underlying new physical concepts of PT symmetric quantum mechanics. In the past, any non-hermitian Hamiltonian was omitted, because it was thought that the corresponding energy eigenvalues are not real. In recent years, the reality of energy spectrum for some non-Hermitian Hamiltonians have been shown. The reality of energy eigenvalues of the trapped particle for a non-Hermitian Hamiltonian has not been investigated up to now.
It may be worthwhile to look for some analytically solvable PT symmetric potentials for the study of reality of energy spectrum of the trapped particle with a non-hermitian Hamiltonian. One of such potentials can be generated by a complex shift of coordinate.

$$V(x) = \omega^2(t)\ (x - ic)^2 + \frac{g}{(x - ic)^2}\ . \tag{16}$$

Shifting the coordinate from x to $z = x - ic$, removes the singularities on the real line, and extends the potential from the half line to the full line. Now, our aim is to investigate the reality of the energy spectrum for this non-Hermitian Hamiltonian. Znojil proved that the energy eigenvalues are real [19, 31] provided that the exact wave function of (16) which vanishes at infinity is used. The eigenvalues and the eigenfunctions of the generalized harmonic oscillator with $\omega^2 = 1$ is given by [19]

$$\Psi_{nq} = N z^{-q\beta+1/2}\ \exp\left(-\frac{z^2}{2}\right) L_n^{-q\beta}(z^2)\ ; \tag{17}$$

$$E_{nq} = 4n + 2 - 2q\alpha\ , \tag{18}$$

where L_n^β are the associated Laguerre polynomials, $(\beta^2 - 1/4 = g)$, $n = 0, 1, 2, ...$ and $q = \pm 1$ is the quasi parity.

The complex extension of the harmonic plus the inverse harmonic potential is of great importance, since it's energy eigenvalues are real as can be seen in the equation (19). However, it is not clear whether the energy eigenvalues remain real for the particle trapped in a box for the non-Hermitian potential (16).

The confined solution of (16) to the equation is obtained from the equation (13) by shifting the coordinate

$$\Psi_\nu(x - ic, t) = N \exp\left(i\alpha \frac{(x - ic)^2}{2} - i \int_0^t dt' \frac{E}{L^2} \right) \frac{1}{\sqrt{L}} R_\nu(x - ic, t) \ . \tag{19}$$

This solution can be compared to the another solution (17) which vanishes at infinity.

For a better understanding, let us use a special value of ν in the Bessel function. If we set $\nu = 1/2$

$$\sqrt{\frac{x - ic}{L}}\ J_{1/2}(\sqrt{E}\ \frac{x - ic}{L}) = \sqrt{\frac{2}{E\pi}} \sin(\sqrt{E}\ \frac{x - ic}{L}) \ . \tag{20}$$

Before investigating the reality of energy spectrum for this wave function, let us check the boundary condition if we shift the coordinate.

The wave function of the physically trapped particle goes to zero at the imaginary points in this case.

$$\Psi_\nu(ic, t) = \Psi_\nu(L + ic, t) = 0 \ , \tag{21}$$

Shifting the coordinate from x to $z = x - ic$ changes also the boundary condition. The new model with complex boundary conditions to describe the trapped particle in non-hermitian quantum mechanics is different from the model used to describe the trapped particle in standard quantum mechanics. However, the reality of the length of the box (quantum dot) is not violated under complex shift of coordinate. It is imposed by the nature that the length of the box must be real like the energy spectrum. In other words, not only the energy eigenvalues but also the length of, say, quantum dot must be real. Although the wave function is set to zero at the complex points describing the locations of the wall of the box, the length of the box is still physical, namely, $\Delta L = L - 0 \rightarrow (L + ic) - (0 + ic) = L$. The reality of the length of the box is preserved with the less strict boundary conditions.

To get a deep understanding of physical implications of confinement in PT symmetric theory,

let us find the absolute square of the wave function by using (20)

$$|R_{1/2}|^2 = \frac{2}{E\pi} \ \sin(\sqrt{E} \ \frac{x-ic}{L}) \sin(\sqrt{E} \ \frac{x+ic}{L}) = \frac{1}{E\pi} \left(\ \cosh(\ \frac{2\sqrt{E}}{L} \ ) - \cos(\ \frac{2\sqrt{E}}{L} x \ ) \right) \ . \tag{22}$$

Trapping of a particle can be modeled using particle in a box perspective. From the experimental point of view, not the wave function Ψ but it's absolute square $|\Psi|^2$ is important. Actually, the probability of finding the particle can be measured at only real points. If we look at (22), we observe that the absolute square of the wave function is not zero at the walls of the box ($x = 0, x = L$). It leads to the non-vanishing boundary conditions for $|\Psi|^2$.

$$|\Psi|^2_{x=0, \ L} \neq 0 \ . \tag{23}$$

This result has crucial implications. A consistent picture of confinement in PT symmetric quantum theory leads to unexpected result. In usual quantum theory, both the wave function Ψ and it's absolute square $|\Psi|^2$ vanish at the wall of the box. When making measurements to find the probability of a trapped particle at the wall of the box, the two theory gives different result.

So far, the case $\nu = 1/2$ have been studied for a better understanding the physical implications. The validity of these results can also be checked for different values of ν .

$$|R_\nu|^2 = \sqrt{\frac{x^2+c^2}{L}} \ J_\nu(\sqrt{E} \ \frac{x-ic}{L}) \ J_\nu(\sqrt{E} \ \frac{x+ic}{L}) \ . \tag{24}$$

Having investigated the boundary conditions, let us now find a relation for the expectation values for the trapped particle in the non-hermitian harmonic oscillator potential.

Instead of calculating the energy eigenvalues directly, our strategy is to start from the energy eigenvalues for the Hermitian Hamiltonian (3) in order to investigate the reality of energy eigenvalues for the non-Hermitian one.

$$\int_0^L \Psi^\star(x) H(x) \Psi(x) dx \in \Re \ , \tag{25}$$

We know that the energy eigenvalues are real for the Hermitian harmonic oscillator potential given by (3) from which the corresponding non-Hermitian Hamiltonian is obtained by the complex shift of the coordinate. If we make a change of variable $x \rightarrow x - ic$ in the above integral, the result of the integration is not changed. Hence, the reality of the integration is

not lost

$$\int_{-ic}^{L-ic} \Psi^\star(x-ic)H(x-ic)\Psi(x-ic)dx \ . \tag{26}$$

The wave function was chosen to be zero at $x = ic, L + ic$ (21). To reach a true expression for the expectation value, let us take the complex conjugate of the above equation.

$$\int_{ic}^{L+ic} \Psi^\star(x-ic)H(x+ic)\Psi(x-ic)dx \ , \tag{27}$$

where we have used $H^\star(x-ic) = H(x+ic)$. We need the relation between $H(x+ic)$ and $H(x-ic)$ to proceed. As a special case, let us find this relation for the case with pure non-Hermitian harmonic oscillator potential ($g = 0$). It is given by $H(x+ic) = H(x-ic) + 4i\omega^2 cx$. Substituting this into the abobe equation, we obtain

$$\int_{ic}^{L+ic} \{\Psi^\star(x-ic)\left(H(x-ic)+4i\omega^2 cx\right)\Psi(x-ic)\}dx \ . \tag{28}$$

$$< E > +4i\omega^2 c \ < x > \in \Re \ . \tag{29}$$

It is a remarkable result that energy and the expectation value of the position operator x can not be real simultaneously for the trapped particle if ω is not zero. The reality of energy eigenvalues is preserved for the trapped particle with the non-Hermitian Hamiltonian only for free particle $\omega^2 = 0$. This is reasonable since the free particle Hamiltonian remains still Hermitian if we shift the coordinate to the complex plane. For the non-vanishing ω, the energy eigenvalues are not real. This is an unexpected result because they are real when the particle is not trapped for the same non-hermitian Hamiltonian [19].

To sum up, the generalized harmonic oscillator plays an important role in understanding the new physical effects of PT symmetric quantum mechanics. We observed the non-vanishing probability density at the wall of the box surrounding the trapped particle. Furthermore, it was shown that energy and the expectation value of x can not be real simultaneously.

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